JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(37), 9672-9679, DOI:10.1021/ja9812397

SUPPORTING INFORMATION

Supporting Information

Conformational Complexity of Succinic Acid and Its Monoanion in the Gas Phase and in Solution: Ab Initio Calculations and Monte Carlo Simulations

Daniel J. Price,[†] John D. Roberts,[‡] and William L. Jorgensen*[,†]

Contribution from theDepartment of Chemistry, Yale University, New Haven, Connecticut 06520-8107, and the Gates and Crellin Laboratories of the California Institute of Technology, Pasadena, California 91125

Supplementary Table 1. OPLS-AA Non-Bonded Parameters for Carboxylic Acids and Carboxylate Anions

Atom	q , e	σ, Å	ε, kcal/mol
Acids			
C	0.520	3.750	0.105
O	-0.440	2.960	0.210
OH	-0.530	3.000	0.170
HO	0.450	0.000	0.000
HC	0.060	2.500	0.030
CT	a	3.500	0.066
Carboxylates			
C	0.700	3.750	0.105
O	-0.800	2.960	0.210
HC	0.060	2.500	0.030
α-CT	b	3.500	0.066
CT	a	3.500	0.066

[a] Assigned to make the CH_n group neutral. [b] Assigned to make the charge on the α- CH_n group = -0.10 e.

Supplementary Table 2. Bond Stretching and Angle Bending Parameters[a]

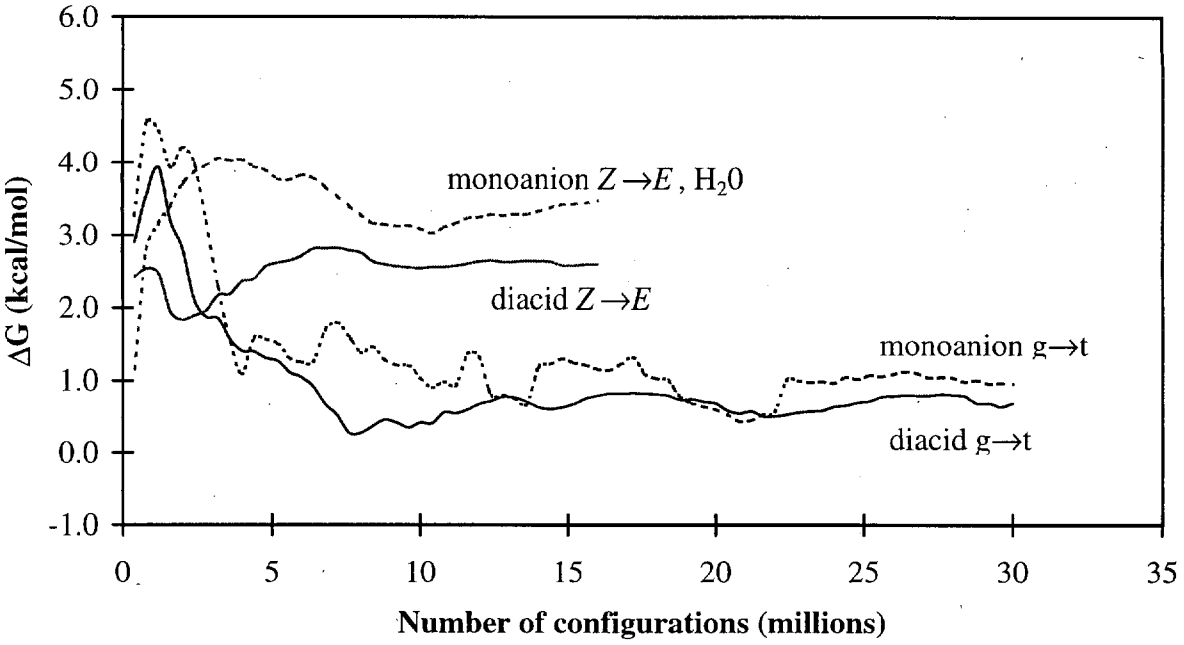
Bond or Angle	k	r_0 or θ_0
CT-CT	268.0	1.529
CT-HC	340.0	1.090
C-CT	317.0	1.522
C-O	570.0	1.229
C-OH	450.0	1.364
OH-HO	553.0	0.945
C-CT-CT	63.0	111.1
C-CT-HC	35.0	109.5
C-OH-HO	35.0	113.0
CT-C-O	80.0	120.4
CT-C-OH	70.0	108.0
CT-CT-HC	37.5	110.7
O-C-OH	80.0	121.0
O-C-O	80.0	126.0

[a] For bonds, k in kcal/mol-Å^2, r_0 in Å. For angles, k in kcal/mol-rad^2, θ_0 in degree

Supplementary Table 3. OPLS-AA Torsional Parameters for Carboxylic Acids and Carboxylate Anions

Angle Type	V_1, kcal/mol	V_2, kcal/mol	V_3, kcal/mol
Acids & Carboxylates			
CT-C-OH-HO	3.000	4.900	0.000
O-C-OH-HO	0.000	4.900	0.000
HC-CT-C-O	0.000	0.000	0.000
HC-CT-C-OH	0.000	0.000	0.000
CT-CT-C-O	0.000	0.546	0.000
CT-CT-C-OH	1.000	0.546	0.450
HC-CT-CT-C	0.000	0.000	0.074
HC-CT-CT-HC[a]	0.000	0.000	0.318
HC-CT-CT-CT[a]	0.000	0.000	0.366
CT-CT-CT-CT[a]	1.740	-0.157	0.279
Monocarboxylates			
CT-CT-C-O	0.000	0.820	0.000
HC-CT-CT-C	0.000	0.000	-0.225
CT-CT-CT-C	-3.185	-0.825	0.493
1,2-Diacids			
CT-CT-C-O	-0.750	-0.550	-0.250
C-CT-CT-C	-0.550	0.000	1.000
1,2-Diacid Monoanions			
CT-C-OH-HO	3.200	4.900	0.000
CT-CT-C-O	-1.000	-1.900	-0.900
C-CT-CT-C	0.800	0.000	0.900

[a] Standard alkane parameters (reference 11).



Supplementary Figure 1. Convergence of the *Z* to *E* and gauche to trans free energy changes from the FEP calculations. The abscissa records the number of Monte Carlo configurations during the averaging periods.

HF/6-31G* optimized structure of the ZsgsZ conformer of succinic acid in Gaussian Z-matrix format.

```
Gaussian Z-matrix ZsgsZ diprotic succinic acid MP2/6-311+G**//HF/6-31G*
E=-455.9529098 au

0 1
 C
 X    1       1.000000
 X    2       1.000000   1     90.000000
 C    1       1.520384   2     90.000000   3      0.000000
 C    4       1.507496   1    112.095989   2      0.000000
 O    5       1.188012   4    125.347101   1     11.052565
 O    5       1.327427   4    111.927674   6    178.389509
 C    1       1.507497   4    112.095967   5     69.166660
 O    8       1.188012   1    125.347142   4     11.052062
 O    8       1.327427   1    111.927652   9    178.390538
 H    7       0.952416   5    108.290759   6     -1.132562
 H    10      0.952416   8    108.290731   9     -1.132066
 H    1       1.081912   4    111.439324   8   -121.734613
 H    1       1.086127   4    110.431307   8    119.463402
 H    4       1.086127   1    110.431277   5    119.463412
 H    4       1.081912   1    111.439326   5   -121.734553
```

HF/6-31+G* optimized structure of the Ecgs conformer of succinate in Gaussian Z-matrix format.

```
Gaussian Z-matrix Ecgs succinate MP2/6-311+G**//HF/6-31+G* MP2
E=-455.4222834 au

0 1
 C
 X    1       1.000000
 X    2       1.000000   1     90.000000
 C    1       1.540236   2     90.000000   3      0.000000
 C    4       1.521219   1    116.308174   2      0.000000
 O    5       1.200654   4    121.572561   1    128.044945
 O    5       1.306279   4    116.725532   6    178.879262
 C    1       1.544473   4    115.943705   3    146.345245
 O    8       1.223141   1    116.486398   4    148.686535
 O    8       1.253989   1    115.816590   9    179.083587
 H    7       0.990952   5    111.058290   6    181.250227
 H    1       1.083663   4    108.865009   8    121.612331
 H    1       1.089319   4    110.026112   8    237.673025
 H    4       1.087456   1    109.215292   5    238.312146
 H    4       1.082810   1    110.106546   5    120.446705
```